

Model Performance

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|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.87 | 0.81 | 0.87 | 0.82 | 0.86 | 0.86 |

Model Results

Predicted value: 3.21e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.97e-01

Confidence level: 7.23e-01

Nearest Neighbors from the Training Set

| | | |
|---|---|--|
| <div>Image not found</div> <div>Dichlorvos</div> <div>Measured: 4.05e-02</div> <div>Predicted: 3.21e-02</div> | <div>Image not found</div> <div>Phosphoric acid, 2-chloroethenyl diethyl ester</div> <div>Measured: 4.66e-02</div> <div>Predicted: 4.25e-02</div> | <div>Image not found</div> <div>Tris(2-chloroethyl) phosphate</div> <div>Measured: 2.45e-02</div> <div>Predicted: 2.74e-02</div> |
| <div>Image not found</div> <div>Phosphonic acid, trichloromethyl-, diethyl ester</div> <div>Measured: 1.76e-02</div> <div>Predicted: 1.93e-02</div> | <div>Image not found</div> <div>Naled</div> <div>Measured: 5.25e-03</div> <div>Predicted: 8.25e-03</div> | |